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MPA Materials Matter

INSIDE

Ulises Martinez, an MPA-11 fuel cell researcher, analyzes a next-generation PGM-free catalyst, a material aimed at significantly reducing the cost of fuel cell technology.
Photo by Michael Pierce (XIT-TSS)

Ulises Martinez

Energized to make a difference

By H. Kris Fronzak, ADEPS Communications

As a member of Materials Synthesis and Integrated Devices' (MPA-11) fuel cell team, Ulises Martinez investigates and refines automotive fuel cells to develop the country's energy options. As a mentor with the Lab's Consortium for Materials and Energy Security, he empowers aspiring students from historically black colleges and universities (HBCUs) to discover their own scientific footing. Both endeavors are fueled by his passion for improving the future.

> *"I try to let my mentees at the Lab and elsewhere know that if they put the work and effort, success is possible, and more importantly, rewarding. If I can do it, they can do it."*

Martinez has taught math and science to high-risk Hispanic high school students; mentored graduate students, and postdoctoral researchers; tutored basic literacy skills to immigrant adults in Santa Fe; introduced disadvantaged schoolchildren to biomaterials, bioengineering, and nanoscience through several outreach programs in Albuquerque; and advised chemical engineer at the University of New Mexico (UNM).

As part of the NNSA-sponsored Consortium for Materials and Energy Security (CMAES), which the Lab has participat-

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From Rick's desk . . .

Time flies by quickly when you are having fun. It is December, the holiday season is underway and it is time to start planning for our next Materials Capability Review. As you know we have our annual review in the spring and we typically focus on at least two of our Areas of Leadership. In last year's review, we provided an update of our Materials Strategy and a deep dive into Manufacturing Science and Integrated Nanomaterials. This year we will provide an overview of all seven leadership areas. With that in mind, this column focuses on the committee's recommendations from last year's review and a brief summary of what to expect.

"The review committee's first recommendation focused on advancing our Materials Strategy to the next level. ... We have taken action on several of the recommendations from the committee."

The review committee's first recommendation focused on advancing our Materials Strategy to the next level. They recommended that we be less aspirational and more vision-oriented and actionable. They also encouraged us to develop an implementation plan with metrics and measurable milestones, and to identify external partners for each leadership area. Its second recommendation suggested building on current efforts to enhance our workforce. They strongly acknowledged the importance of recruiting and retention and recommended we redouble our efforts to attract and retain diverse candidates, while addressing "mid-career malaise." Their third recommendation encouraged us to increase our identification with "one Los Alamos," by working on transparency in communication, increasing efforts to stimulate cross-fertilization across LANL, and balancing group autonomy with institutional uniformity. Its next recommendations focused on the Areas of Leadership featured in the review. Overall the committee was very impressed with our current efforts in Manufacturing Science and encouraged additional outreach, workshops, and engagement with our collaborators both internal and external to LANL. In Integrated Nanomaterials, the committee recognized that our efforts are first rate and recommended that we strengthen and articulate the connection between truly impressive science and LANL mission needs beyond energy security.

We have taken action on several of the recommendations from the committee. The Materials Leadership Team continues to refine our materials strategy. We have released a high-level synopsis, updated websites, and plan to continue to have town hall meetings to better communicate the strategy, objectives, and implementation plan. We are actively engaged with human resources and our institution to address concerns regarding onboarding, mentoring, and leadership development programs. We are also actively participating in surveys to address the Lab's health of science and safety culture. We are proud that this year our LDRD Strategic Investment Plan is more inclusive than in the recent past. And finally, we continue to work across divisions to facilitate cross-organizational teaming and collaborations, and to prioritize investments.

This coming year, our Materials Capability Review will be held April 8-11 and will provide a brief overview and technical talk for each Area of Leadership. We also anticipate several posters for each area. Our goals are to show world-class science in each area and strong connection to our mission, with a demonstrated impact. This is an exciting opportunity to showcase our outstanding science, impact, and relevance to LANL's mission in the areas of Nuclear Deterrence, Global Threat Reduction, and Energy Security. All MPA employees are encouraged to attend and participate, and we welcome your feedback.

Rick

MPA Deputy Division Leader Rick Martineau

“I hope you say hello. I hope you tell me your ideas, and I hope you remember that CINT is always open for collaboration.”

From Andreas’s desk . . .

First, I’ll tell you how I got here. Fourteen years ago I came to the United States and worked in industry for a hard-driving company working on high-density ferroelectric memory and scanning probe microscopy. This satisfied my curiosity for very small things and in this experience I came to appreciate the importance of focused, basic research. Later, when I moved to the R&D department, I was met with a whole new challenge of starting from scratch and bringing new product ideas (memristors and spin-torque MRAM) to the development stage. I then decided to try my hand at running a business and opened a start-up. The unique role that start-ups play in turning an idea into a product is one that has stuck with me. Most recently, I worked at Argonne National Laboratory, working with its nanoscale research center. There I served as deputy director and then acting director and really got to know what the nanoscale research centers (NSRCs) are about. The funny thing about the NSRCs is that their work is solely defined by size. While everyone studies “nanoscale” phenomena, for some this is nanoelectronics, for others chemistry, and yet others biology. Sometimes language becomes an issue, but ultimately the diversity of minds and materials leads to fascinating collaborations. I later transitioned at Argonne from working directly in the nanoscale to starting a new program called Chain Reaction Innovations, which was funded through the Advanced Manufacturing Office to embed entrepreneurs into the national lab.

I never lost the fascination for the nanoscale, so I found myself applying to work with CINT. My background with the NSRCs helped me appreciate how unique CINT is, even among the other NSRCs. CINT is managed by two different labs, which can provide a unique challenge, but it also means we can really do something big for the fields within nanoscience. Further, both are NNSA labs, meaning there are fascinating collaborations possible on either side of the fence. I’m curious and eager to see how CINT can help contribute to each lab’s mission. Finally, as someone who has lived in many cities, I implore you to not forget the beautiful scenery that makes this part of the world special.

Now that I’m here I am looking forward to being part of an ever-expanding network of collaborations. As a user facility, CINT already has the structure and mission to collaborate widely across academia, industry, and within the labs. Often our users take advantage of the expertise and specialized equipment at CINT, but we too are in the market for new knowledge and capabilities. When a scientist in another division develops, e.g., a new measurement capability, we may have users who can benefit from that. When whatever-happens-behind-the-fence happens, we would be happy to explore what that can mean for all of us doing basic science in the uncleared world.

In my short time CINT has already been sharing highly anticipated papers and presentations and we’ve had scientists named fellows of Los Alamos National Lab, the American Physical Society, and the Optical Society, to name a few. These scientists will continue to do exceptional work without a single bit of my “wise leadership,” so I consider my role to help bring them new opportunities. It seems to me that the real point of this write-up is that you get to see the picture of the new guy. So now when you see me, I hope you say hello. I hope you tell me your ideas, and I hope you remember that CINT is always open for collaboration.

CINT Center Leader Andreas Roelofs

Martinez cont.

ed in since 2013, Martinez mentors students from HBCUs, helping them navigate the scientific method and get hands-on research experience. Several of Martinez's mentees have gone on to pursue STEM degrees at UNM, his alma mater.

"For Ulises to be able to convey such a rich science to novices in the field and have them understand it to the point that they want an advanced degree—that's an exceptional skill to have," said Tommy Rockward (MPA-11), the program lead for CMAES.

The consortium hits home for Martinez, who was the first in his family to graduate from college. "I didn't have as much academic support as some, growing up," he said. "I try to let my mentees at the Lab and elsewhere know that if they put the work and effort, success is possible, and more importantly, rewarding. If I can do it, they can do it."

Martinez received chemistry and physics degrees from Indiana's Goshen College in 2004 and continued his studies as a doctoral student in chemical engineering at UNM. Interested in developing technology that didn't depend on fossil fuels, he pursued his PhD with funding from Daihatsu Motor Co., which makes hydrazine fuel cells for automobiles. As part of his doctoral project, Martinez developed several prototypes of an anode catalyst for hydrazine oxidation (please see "Favorite Experiment," below).

Through his PhD advisor, who collaborated with MPA-11 fuel cell team leader Piotr Zelenay, Martinez was aware of the Los Alamos fuel cell program's reputation. Eager to make an impact in fuel cell research, Martinez graduated and applied for a postdoctoral research position at the Lab, discovering through interactions with the fuel cell team a good fit for himself and his goals. He became a staff scientist in 2016.

Martinez focuses on improving fuel cells, primarily through the Department of Energy-sponsored Electrocatalysis Consortium (ElectroCat). The organization aims to boost the durability and speed development of inexpensive platinum group metal-free (PGM-free) fuel cell cathodes. Solving this materials challenge with more durable, carbon-based electrocatalysts for fuel cells could transform the automotive market, enabling this clean power to compete with traditional gasoline engines. Los Alamos co-leads ElectroCat with Argonne National Laboratory.

"The Lab has been at the forefront for a lot of this research, so people look to us for new discoveries," Martinez said. "Though these new catalysts have yet to reach the level of platinum, significant advances have been made to compete with it."

"[Martinez] is helping us on several levels: he's designing and performing his own experiments as well as mentoring students from HBCUs," said Zelenay, who leads the Laboratory's ElectroCat efforts. "It's great to have him here, both as a researcher and a person."

Ulises Martinez's favorite experiment

What: Developed PGM-free nickel-based catalysts for direct-feed (hydrazine) fuel cells in collaboration with Daihatsu Motor Co. for my PhD studies.

Why: NiZn, one of the catalysts I developed, demonstrated mass activities about two orders of magnitude higher than the nickel-only catalyst. It was scaled-up and implemented into the first car prototype powered by direct-feed fuel cells.

When: 2010-2012

Where: University of New Mexico (UNM)

Who: Plamen Atanassov (lead), Barr Halevi, Boris Kiefer, Alexey Serov, Kateryna Artyushkova, and Monica Padilla (University of New Mexico); and Koichiro Asazawa, Tomokazu Sakamoto, and Hirohisa Tanaka (Daihatsu Motor Co.).

How: Boosted activity by alloying of nickel catalyst with a more oxophilic and electron-dense element. Alloying less than 15% zinc with nickel was sufficient to produce a ligand effect in which the nickel's electronic properties were altered by the neighboring zinc. Also, the higher oxophilicity of zinc produced a synergistic catalytic effect by providing required oxygen species to the catalyst-electrolyte interface to remove adsorbed intermediates.

The "aha" moment: The eureka moment was seeing the first prototype of a direct hydrazine fuel cell powered car developed by Daihatsu using a material I had developed. I was fortunate enough to see something go from a catalyst powder I developed in the basement of UNM's chemical engineering building, all the way to the scale-up and implementation in a vehicle.

MPA staff in the news

Htoon, Zapf named 2017 APS Fellows

Han Htoon (Center for Integrated Nanotechnologies, MPA-CINT) and Vivien Zapf (National High Magnetic Field Laboratory-Pulsed Field Facility) were named new American Physical Society (APS) Fellows. To be selected, nominees must have made significant contributions in their respective fields, whether by research, important applications, leadership or service, or education contributions.

Htoon was cited "for pioneering accomplishments in development of single nanostructure, optical spectroscopy/imaging techniques, elucidating fundamental/quantum optical processes of quantum dots and single wall carbon nanotubes, and device integration of optical nanomaterials." He was nominated in the Division of Chemical Physics.

Zapf was cited "for seminal contributions to the understanding of quantum mechanical properties of superconductors, quantum magnets and multiferroic systems at low temperatures and in extreme magnetic fields to 100T." She was nominated in the APS Topical Group on Magnetism.

About Htoon

Htoon earned his PhD in physics from The University of Texas at Austin in 2001. He joined the Lab as a Director's Funded Postdoctoral Fellow and since 2005 has been a staff member at CINT, where he studies nanophotonics and optical nanomaterials. He holds one patent, two LANL Achievement Awards, a Los Alamos Postdoctoral Distinguished Performance Award, and an Achievement Award for Program Development from the Associate Directorate for Chemistry, Life, and Earth Sciences.

About Zapf

After graduating from University of California, San Diego, in 2003 with a PhD in physics, Zapf became a postdoctoral fellow at the California Institute of Technology and then at Los Alamos, as a Director's Funded Postdoctoral Fellow. Since 2006 she has been a staff member at the National High Magnetic Field Laboratory-Pulsed Field Facility, where she focuses on multifunctional and hard magnets, quantum magnetism, inorganic oxide materials, and metal-organic materials. She is the recipient of the 2010 Lee Osheroff Richardson Science Prize and a Los Alamos Distinguished Performance Award.

"Selection as American Physical Society Fellows reflects the vibrant engagement that Los Alamos scientists have with the larger scientific community," said Laboratory Director Charlie McMillan. "I am proud of the contributions Los Alamos scientists bring to professional societies through papers, scientific conference attendance and other professional interactions. Collaboration and the exchange of ideas through affiliations within societies such as APS play an important role in furthering the scientific innovation required to accomplish our national-security mission."

As 2017 APS Fellows, Htoon and Zapf are joined by their LANL colleagues Christopher J. Fontes (Materials and Physical Data, XCP-5), Toshihiko Kawano (Nuclear and Particle Physics, Astrophysics, and Cosmology, T-2), John W. Lewellen (Accelerators and Electrodynamics, AOT-AE), Laura Beth Smilowitz (Physical Chemistry and Applied Spectroscopy, C-PCS), and Stuart A. Trugman (Physics of Condensed Matter and Complex Systems, T-4). The APS, a nonprofit membership organization formed in 1899 to advance and spread the knowledge of physics, represents more than 51,000 members worldwide and publishes more than a dozen scientific journals.

Technical contacts: Han Htoon and Vivien Zapf

Mohite named 2017 Resonate Award winner

Aditya Mohite (Materials Synthesis and Integrated Devices, MPA-11) is the 2017 Resonate Award Winner, presented by faculty in the California Institute of Technology Resnick Sustainability Institute. He was cited for developing two-dimensional and thin-film materials for high-performance solar electricity generation. The Resonate Award honors outstanding achievement in renewable energy and sustainability-focused science and technology. It aims to highlight up-and-coming innovators who have made new contributions to sustainability science, particularly in energy security, climate change, and the environment.

Mohite, an expert in device physics and material science who joined the Laboratory in 2009 as a postdoctoral researcher in the Center for Integrated Nanotechnologies (MPA-CINT), directs an energy and optoelectronic devices lab at Los Alamos and leads the Light to Energy team. His research focuses on understanding and controlling charge and energy transfer processes occurring at interfaces created with organic and inorganic materials for thin-film clean energy technologies. He develops creative approaches to

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MPA staff cont.

Aditya Mohite (right) accepts the 2017 Resonate Award from Resnick Institute Director Jonas Peters.

solve fundamental scientific issues and to enable devices to perform as well as or better than current technology. His work supports the Laboratory's Energy Security mission and its Materials for the Future science pillar.

Mohite, who earned his PhD in electrical engineering from The University of Louisville in 2007, has published more than 100 peer-reviewed papers and delivered more than 75 invited talks. He works to find innovative and out-of-the-box concepts and solutions for the next generation of clean energy advances. Achieving this requires an in-depth understanding and control of physical properties across multiple scales at relevant operating conditions. These strategies have translated to high performance devices with the stability required to be useful in the real world.

The Resnick Sustainability Institute draws on the California Institute of Technology's legacy of innovation, seeking to empower next-generation pioneers by recognizing their contributions to sustainability across all sciences and technology. The award was given at a special reception as part of the school's 2017 Resnick Young Investigators Symposium, which celebrates young researchers who have established science and engineering initiatives that show promise in tackling sustainable future challenges.

Technical contact: Aditya Mohite

Celebrating service

Congratulations to the following MPA Division employees celebrating recent service anniversaries:

Jeff Willis, MPA-11	40 years
Geraldine Purdy, MPA-11	30 years
George Rodriguez, MPA-CINT	25 years
Rod Borup, MPA-11	20 years
James Werner, MPA-CINT	20 years
Sergei Ivanov, MPA-CINT	15 years
Doan Nguyen, NHMFL-PFF	10 years

MPA innovations chosen as R&D 100 Award winners

Two technologies developed, in part, by Materials Physics and Applications (MPA) researchers, were named 2017 R&D 100 Awards. The awards honor the top 100 proven technological advances of the past year, and are determined by a *R&D Magazine* panel.

Clean-Energy Electrocatalysts Without Precious Metals, created by researchers from Materials Synthesis and Integrated Devices (MPA-11), Sigma Division (Sigma-DO), and collaborators at Pajarito Powder, LLC, uses inexpensive materials to synthesize electrocatalysts for hydrogen fuel cells. These new, precious-metal-free electrocatalysts offer performance approaching that of precious metal catalysts but at a fraction of the cost, with a much higher tolerance to virtually all contaminants and impurities common to the fuel cell hardware, hydrogen, and air feed stream. Applications include transportation, portable batteries, and stationary emergency backup power.

Clean-Energy Electrocatalysts Without Precious Metals was jointly submitted with Pajarito Powder, and is based on technology that Pajarito Powder licensed from the Lab. Piotr Zelenay (MPA-11) led the Los Alamos team of Edward Holby (Sigma-DO) and Hoon Taek Chung and Ulises Martinez (both MPA-11). Pajarito Powder collaborators include Barr Zulevi, Alia Lubers, Geoff McCool, and Sam McKinney. Hydrogen Safety Sensor is designed to make filling up hydrogen-fueled vehicles significantly safer. Hydrogen gas is highly flammable, colorless, odorless, and quickly propagated if released. The Hydrogen Safety Sensor uses durable, long-lasting ceramic sensor elements that can be placed anywhere in the hydrogen supply chain—from hydrogen production to the "pump" at a filling station, and the consumer product.

The device was created and submitted to the awards with collaborators Lawrence Livermore National Laboratory (LLNL) and Hydrogen Frontier, Inc. Testing at Hydrogen Frontier filling stations showed that the sensors are highly sensitive and selective to hydrogen with no baseline drift or false alarms. This sensor could benefit all facets of the hydrogen economy, from transportation to hydrogen generators and off-grid power sources.

Eric Brosha led the Los Alamos team of Christopher Romero, Rangachary Mukundan, and Cortney Kreller (MPA-11).

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R&D 100 Awards cont.

Collaborators on Hydrogen Safety Sensor include Amanda Wu and Robert Glass (LLNL) and Daniel A. Poppe (Hydrogen Frontier).

Eight Los Alamos National Laboratory innovations—ranging from energy to health, modeling and simulation, materials, and engineering—were named winners in the prestigious "Oscars of Invention," which span industry, academia, and government-sponsored research organizations. Since 1978, Los Alamos has won 145 R&D 100 Awards.

"The R&D 100 Awards represent the breadth, depth and innovation of the science and engineering at our Laboratory. They also reflect our partnerships with other government laboratories, universities and private industry," said Los Alamos National Laboratory Director Charlie McMillan. "These innovations continue the Laboratory's tradition of scientific excellence in support of our national security mission and to the broader scientific community. I congratulate the teams on their outstanding achievements."

Technical contacts: Eric Brosha, Piotr Zelenay

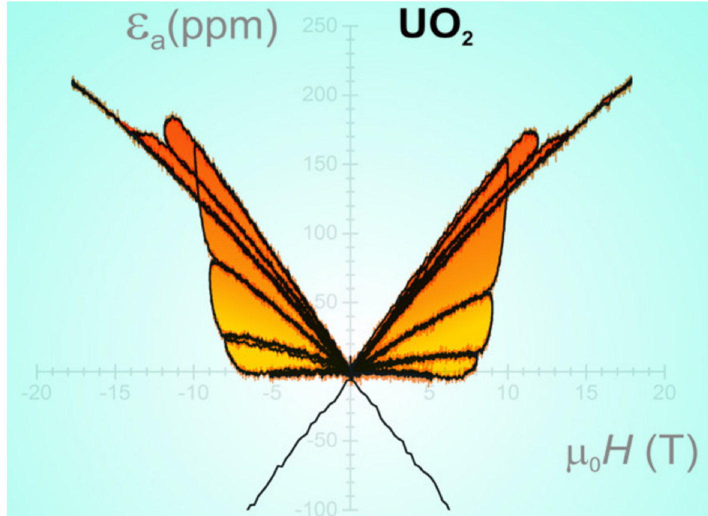
Study of uranium dioxide properties improves understanding of essential nuclear power plant fuel

By exploring the magnetic and crystal lattice properties of uranium dioxide (UO_2), researchers at Los Alamos and Idaho national laboratories and at the Aix-Marseille University in France are improving understanding of an essential nuclear power plant fuel. The research, published in *Nature Communications*, details magnetoelastic properties of UO_2. The interplay between the material's lattice structure and its magnetic properties may have important implications for its thermal properties, especially thermal conductivity.

Antiferromagnetism sets in below T_N = 30K, and record high magnetic fields were used to probe the material's unusual resilience, which is believed to be linked to its strong entanglement with the crystal lattice. The work marks the first low-temperature magnetostriction study of UO_2 in magnetic fields up to 92.5 tesla.

Better understanding of UO_2's lattice properties, critical to get a grasp on the reasons behind its crippled thermal conductivity, could aid the development of new fuels and models of the material properties. Further research in these areas could lead to safer and more economic reactor design, which is an important part of DOE missions.

Using single-crystal samples of UO_2, the team tested the material's magnetoelastic properties in record high magnetic fields at the National High Magnetic Field Laboratory's Pulsed Field Facility. This, coupled with computational



A strain hysteresis butterfly for UO_2 in magnetic fields to 20T, which was measured at the National High Magnetic Field Laboratory-Pulsed Field Facility.

research, showed tiny distortions in the crystals' cubic shape at the core of piezomagnetism. These distortions switched along with the polarity of high magnetic fields up to 92.5 Tesla. The study also discovered first-order coupling between the magnetism in U-atoms and lattice degrees of freedom, which could be the origin of scattering of phonons against spin fluctuations dressed with dynamic Jahn-Teller oxygen modes well above T_N.

The Pulsed Field Facility, supported by DOE, the National Science Foundation (NSF), and the State of Florida, is the only facility in the world capable of generating record-breaking magnetic fields to 100T in a nondestructive fashion. Los Alamos research was supported by the NSF, DOE Office of Basic Energy Sciences, and the State of Florida through a NSF cooperative grant. The work supports the Laboratory's Energy Security mission area and its Materials for the Future science pillar.

Researchers: Marcelo Jaime, Myron Salamon, Vivien S. Zapf, and Neil Harrison (National High Magnetic Field Laboratory-Pulsed Field Facility); A. Saul (Aix-Marseille University, France); Tomasz Durakiewicz (Condensed Matter and Magnet Science, MPA-CMMS and Maria Curie-Sklodowska University, Poland); Jason C. Lashley (Materials Synthesis and Integrated Devices, MPA-11); D. A. Andersson and Chris R. Stanek (Materials Science in Radiation and Dynamics Extremes, MST-8); James L. Smith (Sigma Division); and K. Gofryk (Idaho National Laboratory).

Reference: "Piezomagnetism and magnetoelastic memory in uranium dioxide." *Nature Communications* **8**, (2017).

Technical contact: Marcelo Jaime

Electronic in-plane symmetry breaking at field-tuned quantum criticality in $CeRhIn_5$

Common phenomenon could be key to understanding mechanism of unconventional superconductivity

F-electron materials have a different hierarchy of energy scales than is found in transition metal and organic materials, but they often have similar complex and intertwined physics coupling spin, charge, and lattice degrees of freedom. Therefore, the ability to find similarities and differences among these classes of materials with novel emergent phenomena helps researchers establish the essential ingredients that cause novel functionalities such as superconductivity.

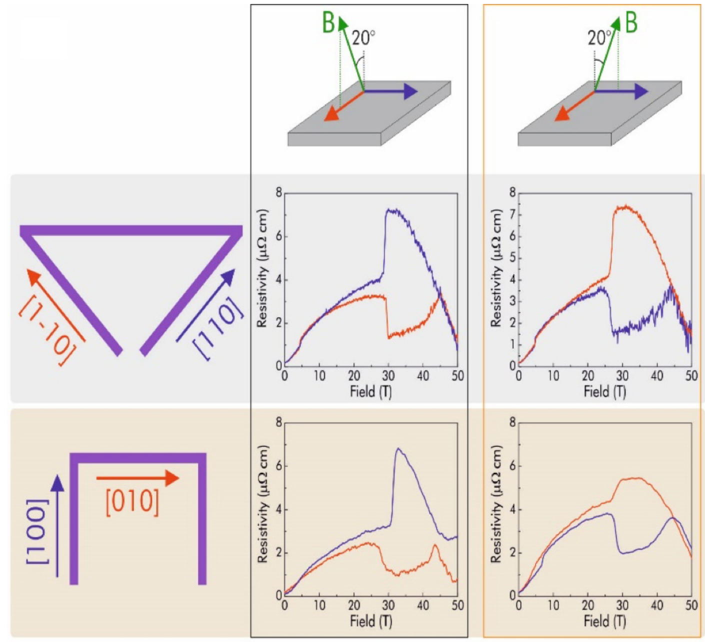
In such an investigation published as a letter in *Nature*, Materials Physics and Applications researchers and collaborators discovered that the high field state of the heavy fermion superconductor $CeRhIn_5$ possesses an electronic nematic, which is a similar symmetry-breaking state as occurs in other unconventional superconductors. Their work reveals a commonality that should be captured by any theories describing unconventional superconductivity on the border of magnetism.

$CeRhIn_5$ is an antiferromagnet at 4 K. Under pressure the magnetism is suppressed giving rise to a dome of unconventional superconductivity, with a large superconducting transition temperature as also occurs in the transition metal cuprate and iron-based superconductors. The latter systems have recently displayed charge and nematic responses, whose relationship to the superconducting state is not understood.

Using transport measurements near the field-tuned quantum critical point of $CeRhIn_5$ at 50 Tesla, the researchers observed a fluctuating nematic-like state. A nematic state is most well known in liquid crystals, wherein the molecules of the liquid are parallel (broken rotational symmetry) but not arranged in a periodic array (no translational symmetry). Nematic-like states have been observed in transition metal systems near magnetic and superconducting phase transitions. The occurrence of this property points to nematicity's correlation with unconventional superconductivity.

The use of the National High Magnetic Field Laboratory's magnets was essential due to the large magnetic fields required to access this state, as was the fabrication of micron sized devices using focused ion-beam milling to enable the transport measurements in large fields.

The work showed there was negligible response in magnetization and lattice degrees of freedom, but a clear change in the symmetry of the electronic degrees of freedom at the same time when a change in the Fermi surface occurs. The in-plane rotational invariance of the symmetry breaking (i.e., the similarity of the response in the B_{1g} and B_{2g} symmetry



Carefully aligned microstructured devices of $CeRhIn_5$ enabled high field transport measurements that reveal an in-plane symmetry breaking for magnetic fields of approximately 30T along the tetragonal c-axis. The anomaly size and direction is determined by a small in-plane component of the magnetic field.

channels) in $CeRhIn_5$ is a novel feature among systems displaying a nematic response, and distinguishes the response in $CeRhIn_5$ as an XY-nematic as opposed to an Ising type nematic.

The research supports the Lab's Energy Security mission area and its Materials for the Future science pillar. It was sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, the Max Planck Society, and the Deutsche Forschungsgemeinschaft (German Research Foundation). Work at the National High Magnetic Field Laboratory was supported by National Science Foundation Cooperative Agreement no. DMR-1157490, the State of Florida, and the US DOE. M.J. acknowledges support from the IMS Rapid Response program at Los Alamos.

Reference: "Electronic in-plane symmetry breaking at field-tuned quantum criticality in $CeRhIn_5$," *Nature* letter, (2017).

Researchers: Filip Ronning (Condensed Matter and Magnet Science, MPA-CMMS); Toni Helm, Kent Shirer, Maya Bachmann, and Philip J.W. Moll (Max-Planck-Institut for Chemical Physics of Solids - Dresden); Luis Balicas (Florida State University); Mun K. Chan, Brad J. Ramshaw, Ross D. McDonald, Fedor F. Balakirev and Marcelo Jaime (National High Magnetic Field Laboratory-Pulsed Field Facility), and Eric D. Bauer (MPA-CMMS).

Technical contact: Filip Ronning

Atomic-level observations show exactly how low-cost fuel cell catalysts work

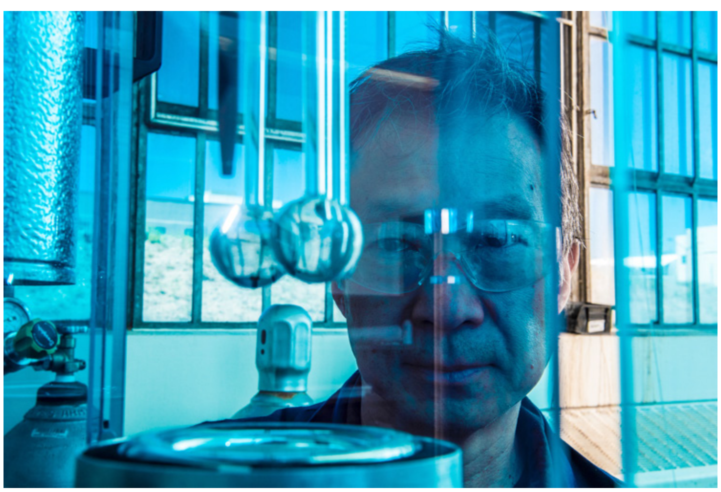
Study aids efforts to find alternatives to expensive platinum-based catalysts

To reduce the cost of next-generation polymer electrolyte fuel cells for vehicles, researchers have been developing alternatives to the prohibitively expensive platinum and platinum-group metal (PGM) catalysts currently used in fuel cell electrodes. A study by Los Alamos researchers and collaborators at Oak Ridge National Laboratory (ORNL), appearing in *Science*, accelerates those efforts by determining efficient new materials and discovering how they work at an atomic level.

Building on previous studies, the Los Alamos-led team synthesized oxygen reduction reaction (ORR) catalysts made of low-cost platinum alternatives that perform comparably to the standard PGM fuel cell catalyst used in vehicle applications. Using sophisticated microscopy at ORNL, scientists for the first time directly observed the single-atom active sites in the novel material where catalysis takes place, therefore providing unique insights into the potential efficiency of this PGM-free material.

The new material used in this study is an iron-nitrogen-carbon (Fe-N-C) fuel cell cathode electrocatalyst, synthesized with two nitrogen precursors that expose much of the carbon surface to oxygen. Significantly, this material's fuel-cell performance is approaching that of platinum catalysts, as shown in fuel cell test-stand performance.

Computer modeling conducted at Los Alamos predicted the high activity of Fe-N-C catalysts, the FeN_4 active-site structure, and the possible reaction pathway, confirming that the sites observed by microscopy are likely responsible for the high ORR activity of the synthesized catalyst.



Researcher Hoon Chung stands behind a Quantachrome Instruments Autosorb iQ_2 gas sorption analyzer, an instrument that measures the surface area and pore-size distribution in fuel cell electrocatalysts

Los Alamos research into fuel cells expands options for energy production, supporting the Laboratory's energy security mission and the Lab's Materials for the Future science pillar.

This work was supported by the DOE Office of Energy Efficiency and Renewable Energy's Fuel Cell Technologies Office. Computational resources were provided by LANL's Institutional Computing program. Researchers include Hoon T. Chung and Piotr Zelenay (MPA-11); Drew Higgins (formerly LANL, now a postdoctoral researcher at Stanford University); David A. Cullen, Brian T. Sneed, Karren L. More (Oak Ridge National Laboratory); and Edward F. Holby (Sigma Division, Sigma-DO).

Reference: "Direct atomic-level insight into the active sites of a high-performance PGM-free ORR catalyst." *Science*, **357** (2017).

Technical contact: Piotr Zelenay

Single-photon emitter has promise for quantum info-processing

First known material capable of single-photon emission at room temperature and at telecommunications wavelengths

Center for Integrated Nanomaterials researchers and collaborators have produced the first known material capable of single-photon emission at room temperature and at telecommunications wavelengths. These carbon nanotube quantum light emitters may be important for optically-based quantum information processing and information security, and are of significant interest for ultrasensitive sensing, metrology and imaging needs and as photon sources for fundamental advances in quantum optics studies.

By chemically modifying a nanotube surface to controllably introduce light-emitting defects, the researchers developed carbon nanotubes as a single photon source. The work, reported in *Nature Photonics*, is a step toward implementing defect-state quantum emitters operating at room temperature and demonstrating their function in technologically useful wavelengths.

Ideally, a single photon emitter will provide both room-temperature operation and emission at telecom wavelengths, but this has remained an elusive goal. Up to now, materials that could act as single photon emitters in these wavelengths had to be cooled to liquid helium temperatures, rendering them much less useful for ultimate applications or scientific purposes.

A critical breakthrough in the nanotube work was the ability of the team to force the nanotube to emit light from a single point along the tube, only at a defect site. The key was to

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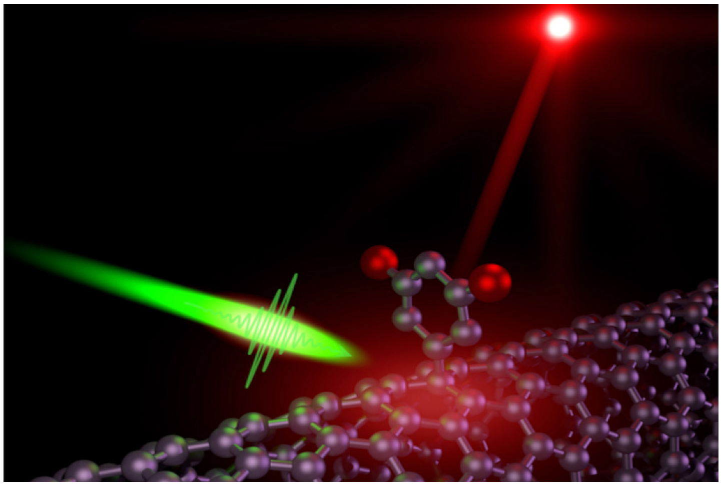
Emitter cont.



CINT researchers and collaborators have produced functionalized carbon nanotubes capable of single-photon emission at room temperature and at telecommunications wavelengths. This artists rendition depicts a carbon nanotube functionalized with a dichlorobenzene molecule to create a single light-emitting defect site. Upon excitation with a pulsed laser (green), a single photon (red) is emitted from the defect site.

limit defect levels to one per tube. By emitting one photon at a time, the photon's quantum properties can be controlled for information storage, manipulation, and information transmission.

The researchers attained this control using diazonium-based chemistry, a process which binds an organic molecule to the nanotube's surface to serve as the defect. The diazonium reaction chemistry allowed a controllable introduction of benzene-based defects with reduced sensitivity to natural fluctuations in the surrounding environment. Importantly, the versatility of the diazonium chemistry also permitted the researchers to access the inherent tunability of nanotube emission wavelengths.

Carbon nanotubes as single photon sources are in their infancy, but developments by the CINT team are enabling significant advances in capability. These functionalized carbon nanotubes have significant prospects for further development in functionalization chemistry; integration into photonic, plasmonic, and metamaterials structures for further control of quantum emission properties; and implementation into electrically driven devices and optical circuitry for diverse applications.

This research was funded in part by the Laboratory Directed Research and Development program and performed at the Center for Integrated Nanotechnologies, a DOE Office of Science User Facility operated jointly by Sandia and Los Alamos national laboratories. It supports the Lab's Global Security mission and its Materials for the Future science pillar in the emergent phenomena thrust, which is part of the Laboratory's scientific pursuit of controlled materials functionality.

Reference: "Tunable room-temperature single-photon emission at telecom wavelengths from sp^3 defects in carbon nanotubes," *Nature Photonics* (2017).

Researchers: Xiaowei He, Nicolai F. Hartmann, Xuedan Ma, Younghee Kim, Han Htoon and Stephen K. Doorn (Center for Integrated Nanotechnologies, MPA-CINT); Rachelle Ihly and Jeffrey L. Blackburn (National Renewable Energy Laboratory); Weilu Gao and Junichiro Kono (Rice University); and Yohei Yomogida, Atsushi Hirano, Takeshi Tanaka and Hiromichi Kataura (National Institute of Advanced Industrial Science and Technology, Japan).

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Consortium aims to strengthen, diversify the country's national security science workforce

A Los Alamos National Laboratory-led effort to diversify the scientific workforce at national laboratories is creating an ever-widening pipeline of minority students passionate about materials and energy research.

The Consortium for Materials and Energy Security (CMaES) is an association of Los Alamos and Lawrence Livermore national laboratories and eight minority-focused colleges and universities providing students with a range of scientific research experiences. Laboratory researchers have mentored 60 students since CMaES' founding. Many students have gone on to attend graduate school, and some are now working full-time at Los Alamos, including in Materials Physics and Applications and Chemistry divisions, making essential contributions to the Lab's national security science mission.

"To find the best STEM [science, technology, engineering, and math] researchers for the next generation, we need to look everywhere," said Los Alamos fuel cell researcher Tommy Rockward (Materials Synthesis and Integrated Devices, MPA-11), who originally proposed the project to the National Nuclear Security Administration (NNSA) to provide additional talent pools and help diversity efforts in laboratory settings. "CMaES and other programs have allowed more students from underrepresented schools to experience national labs. The consortium is becoming a hub for Lab scientists and staff to find talent."

For example, 38% of the African-American students who joined Los Alamos over the last several years originally participated in CMaES, which is part of the Lab's African American Partnership Program.

CMaES gives students hands-on experience in performing scientific research, interpreting data, and writing and presenting reports. In short it prepares them with the necessary skills for a future in science at a national laboratory. Part of its success is due to the program's flexibility in providing students the opportunity to execute research projects on similar equipment whether while attending class or working at a national laboratory.

continued on next page

Consortium cont.

Recent CMaES students gather in a fuel cell lab at Los Alamos. Standing, from left: Andre Spears (graduate student, MPA-11), mentor Joseph Dumont (Chemical Diagnostics and Engineering, C-CDE), Raluchukwu Onwubuya (post baccalaureate student, formerly with MPA-11) Ling Lin (visiting student from University of Science and Technology of China), Oscar McClain (post baccalaureate student, formerly with MPA-11), and mentor Ulises Martinez (MPA-11). Seated, from left: Jonalyn Fair and Courtland Brown (both post baccalaureate students, formerly with MPA-11).

It was initially funded by the NNSA and Los Alamos National Laboratory's Director's Office, but as the program flourished it has gained support from the DOE's Fuel Cell Technology office. Livermore joined CMaES in 2013, giving students a second laboratory setting in which to learn skills and explore career possibilities.

Students, who are recruited from minority-focused institutes, can get involved via three-day "short courses" in a specific subject, summer internships, and year-long stints. The CMaES Bridge Program places students in one-year appointments at Los Alamos or Livermore. During that time, they are required to apply to graduate school and start research that typically extends into thesis work. Another program, the Los Alamos Dynamics Summer School, has supported CMaES students by pairing them with multidisciplinary Los Alamos researchers for nine-week materials projects spanning electrical, mechanical, structural and cyber-physical systems. Students gain professional experience by presenting their results at an international conference.

"I really appreciate the opportunity and the exposure I've gotten through the Lab," Nia Parker, a post-baccalaureate CMaES student in MPA-11 who plans to enroll in a doctoral program in organic chemistry. "The more knowledgeable I am about the world and the science community, the better." In MPA-11, Parker is studying disorder and transport in irradiated pyrochlore thin films.

"Deciding to come to Los Alamos was one of the greatest decisions I could have made. I have always known I wanted to attend graduate school; being at LANL has provided me with more ways to achieve that goal," said Shaylynn Crum (Chemical Diagnostics and Engineering, C-CDE), who joined CMaES as a summer student and is now a post-baccalaureate student developing an additively manufactured polymer with specific structure and characteristics. Crum also assists her group on characterization and infrared spectroscopy projects. Both she and Parker are partly funded through the Director's Office.

Rockward said CMaES and similar programs run by Los Alamos and partner laboratories have allowed more students from underrepresented schools to experience the national lab setting, and given the Labs new locations from which to recruit. He plans to expand the program further by inviting more schools and students to participate.

HeadsUP!

Your MPA Division WSST is…

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The MPA Division WSST meets on the third Tuesday of every month, typically at 11 a.m. in TA-03, Bldg. 1415, conference room 102. WSST meetings are open to everyone. You are invited to attend and share your safety and security concerns and suggestions.

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